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A flexible, integrated system for generating meteorological surfaces derived from point sources across multiple geographic scales

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Abstract

The generation of meteorological surfaces from point-source data is a difficult but necessary step required for modeling ecological and hydrological processes across landscapes. To date, procedures to acquire, transform, and display meteorological information geographically have been specifically tailored to individual studies. Here we offer a flexible, integrated system that employs a relational database to store point information, a modular system incorporating a choice of weather data interpolation methods, and a matrix inversion method that speeds computer calculations to display information on grids of any specified size, all with minimal user intervention. We demonstrate the power of this integrated approach by cross-validating projected daily meteorological surfaces derived from ~1200 weather stations distributed across the continental United States for a year. We performed cross-validations for five meteorological variables (solar radiation, minimum and maximum temperatures, humidity, and precipitation) with a truncated Gaussian filter, ordinary kriging and inverse distance weighting and achieved comparable success among all interpolation methods. Cross-validation computation time for ordinary kriging was reduced from 1 h to 3 min when we incorporated the matrix inversion method. We demonstrated the system's flexibility by displaying results at 8-km resolution for the continental USA and at one-degree resolution for the globe.

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1. Introduction

Although landscape modeling of ecological and hydrological processes commonly requires a similar set of meteorological variables, a challenge exists in gathering information from point-data sources and generating from these a reasonable interpolation or extrapolation across topographically variable conditions at a variety of temporal and spatial scales. Environmental modeling is scale independent ranging from small watershed studies at fine resolutions (Band et al., 1993; White and Running,

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1994) to global studies at course resolutions (Nemani et al., 2003a). Meteorological data for these types of simulations are rarely available at the appropriate spatial or temporal scale (Cramer et al., 1999; Eagleson, 1986; Mummery and Battaglia, 2002).

To date, most modeling exercises have required the development of a processing technique that must be modified extensively to handle different sets of meteorological data, their interpolation or extrapolation, and display at a specified temporal and spatial scale. We recognize, as do others (Baron et al., 1994; Pierce and Running, 1995), that a flexible, more integrated system would be highly desirable and that such a system must be able to acquire and store, transform, and display meteorological information in an efficient, accurate

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manner at multiple geographic scales without extensive user intervention. We envision three discrete components that must be integrated.

The first system component involves data acquisition and storage. If we store point-source observations in a relational database with an *open standard interface* we can remain independent of any specific database management system. We can then use this relational database as a foundation to develop scaleable applications that use data efficiently while still providing point-source data access to nearly any data-aware program. The acquisition and storage of highly variable meteorological data can be done efficiently by incorporating a relational format using *structured query language* (SQL). SQL provides a simple, common interface to allow spatial and temporal selection and summarization of data with ease and efficiency.

The second system component involves the incorporation of techniques to transform point-source weather data into continuous variables that can be displayed spatially. Many applications have tailored interpolation processes specifically for generating surfaces of weather data (Daly and Neilson, 1994; Fleming et al., 2000; Goovaerts, 2000; Hutchinson, 1998; Jeffrey et al., 2001; Price et al., 2000; Thornton et al., 1997). These applications use a variety of mathematical techniques, such as Ordinary Kriging, truncated Gaussian filters or thin plate smoothing splines, but all have the same goal: to generate surfaces of weather data over large spatial scales. We should adapt a modular framework to allow for the substitution of one technique for another without affecting the format of the acquired data or the products generated. Modularity promotes system flexibility and adaptation to changing research needs at different scales (Voinov et al., 2004).

The third system component involves the display of meteorological surfaces at any selected spatial scale. Earth science applications are focusing on modeling processes at multiple scales in near real time (Nemani et al., 2003b) and such a system must be able to efficiently generate meteorological data over a comparable spatial extent. Using inputs of the wrong spatial scale can significantly bias model predictions (Pierce and Running, 1995). We offer in this paper the application of such a flexible system based on criteria provided by the user to the mathematical processor that can generate meteorological data surfaces at any spatial scale.

Briefly, we automatically retrieve and store meteorological data in an SQL database, interpolate those data using a variety of mathematical techniques and display the results over multiple spatial extents. We test the system by implementing three different mathematical processors that interpolate meteorological point-source data: ordinary kriging, a truncated Gaussian filter, and inverse distance weighting and compare the results of these three processors using ~1200 daily station

observations over the continental United States for 2002. We illustrate the advantages of an integrated system by presenting daily meteorological data interpolated across the United States at 8-km resolution on the continent and at one-degree grids at the global scale. We contend that these characteristics culminate in a system that can rapidly adapt to meet the meteorological data needs of environmental modelers.

2. Methods

2.1. Surface observations gridding system (SOGS)

We named the flexible, integrated system that we developed the surface observation gridding system (SOGS). A flow diagram of the system is shown in Fig. 1 that indicates its modular design and functional relationships between data acquisition, storage, interpolation and projection as surface variables on multiple spatial scales.

2.2. Data retrieval and storage

We obtained daily global weather data (Global Surface Summary of the Day) from the National Climate Data Center (NCDC). The system automatically retrieves the most current data from the World Wide Web and stores these data in the relational database. Currently, these summaries are updated by the NCDC about weekly and provide daily observations of maximum, minimum, average and dewpoint temperatures, and precipitation for approximately 6000 global stations. Observations are available from late 1994 to the present. New data sources can be added simply by creating and populating new database tables based on the new data formats and all data can be merged into a superset data source using SQL for use in the interpolation system. An example set of daily global observations from NCDC is shown in Fig. 2.

2.3. Interpolation

The interpolation routine was designed to be *modular* such that the interface to the routine remains the same while the technique itself could easily be switched to use another method. The interpolation routine requires a set of spatially explicit input observations and the location and elevation of the prediction point. It generates a prediction from these inputs. This ensures that other methods can be added with minimal effort. A flow diagram of the modular interpolation logic is shown in Fig. 3. In all cases, locations are specified as longitude (x) (decimal degrees), latitude (y) (decimal degrees) and

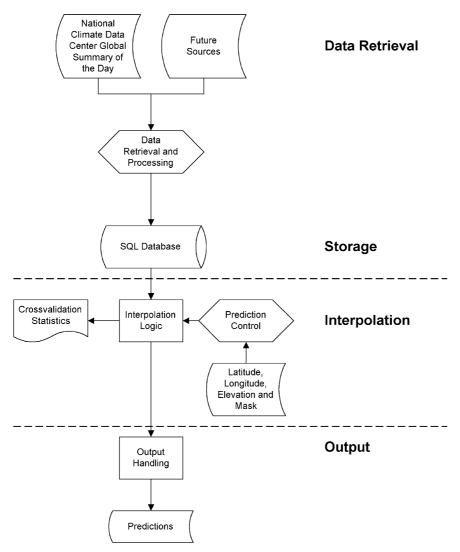


Fig. 1. Flow diagram of the SOGS. Three main components that comprise the system are: data retrieval and storage, interpolation and output handling. Data retrieval is configured to automatically retrieve the most recent data available and insert those data into the SQL database. Interpolation methods are modular and allow maximum flexibility in implementing new routines as they become available. Outputs are generated on the prediction grid that is determined by the latitude, longitude, elevation and mask layers.

elevation (z) (meters). Elevation is explicitly considered as a third dimension due to the covariance of many weather variables with changes in elevation (Barry and Chorley, 1998).

2.4. Generating products

Output generation is linked to the prediction grid using four raster inputs: latitude, longitude, elevation and a simulation mask. The simulation mask determines the presence or absence of a prediction point. Longitude, latitude and elevation layers determine the location and topography of the prediction point, respectively. Although latitude and longitude are used in this example, it is still possible to use other grid coordinates such as UTM. Prediction points outside the region of interest determined by the simulation mask are

not estimated and are set to a fill value. To assess the ease with which new spatial resolutions could be modeled, we generated two test input raster sets: one for the continental United States at eight kilometer resolution and one for the globe at one degree resolution and used these test inputs to interpolate example raster weather data images at those resolutions for May 4th, 2003.

2.5. Interpolation implementation

To test the modularity of the system, we implemented ordinary kriging (OK) (Brooker, 1979), a truncated Gaussian filter (TGF) (Thornton et al., 1997) and inverse distance weighting (IDW) (Isaaks and Srivastava, 1989) as interpolators within the SOGS framework. OK calculates predictions using two components: a matrix

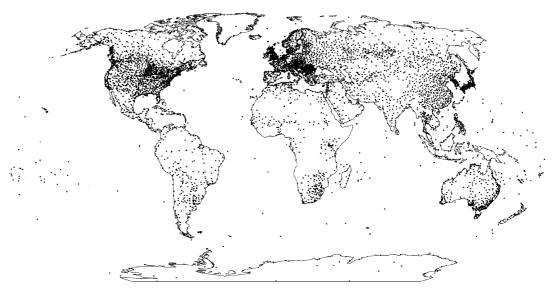


Fig. 2. Sample set of global, daily observations from the NCDC Global Surface Summary of the Day for May 4th, 2003.

of covariances between observations and a matrix of covariances between the observations and the prediction point. These covariances were determined from a spherical semivariogram model. TGF does not consider the covariances between observations, weighting each observation's contribution to the prediction only by its distance to the prediction. It assesses each station's contribution by a Gaussian weighting function that is truncated at some distance from the prediction point. Inverse distance weighting is similar to TGF except that it weighs the contribution of each observation by the squared reciprocal of its distance to the prediction point. The IDW method truncates observations at some distance from the prediction point in the same way as

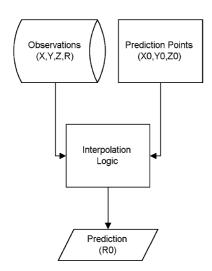


Fig. 3. System flow diagram for modular interpolation logic used in SOGS. Prediction locations (X_0, Y_0, Z_0) and observed data $(X_{1..n}, Y_{1..n}, Z_{1..n}, R_{1..n})$ are input into the interpolation routine and that routine generates a prediction (R_0) based on the observed data and some weighting scheme.

TGF. Specific details for each of the key weather variables interpolated are detailed below.

Because we are interested in optimizing speed and performance, the run was accomplished using identical model parameters for each respective method for all five variables. This allowed the calculation of a single observation weight for all interpolated variables. Fixing model parameters also ensures that the same observations are included for each method for each prediction. Each method has a truncation distance and if these were allowed to vary, different numbers of observations would be allowed for each prediction with each method, possibly confounding the comparison of the three interpolators. Fixing these parameters therefore allows for a more direct comparison between the methods. These fixed model parameters for each of the methods are shown in Table 1.

Table 1 Model parameters for ordinary kriging, the truncated Gaussian filter and inverse distance weighting implemented in SOGS

and inverse distance weighting implemented in 50 ds				
_				
10.0				
5.5°				
0.0				
6.5				
5.5°				
2.0				
5.5°				

Range and truncation radius parameters are in decimal degrees. Variogram sill and nugget values are in variance units of either ${}^{\circ}C^2$ for temperatures, (W m $^{-2}$) 2 for solar radiation and cm 2 for precipitation. The truncated Gaussian filter shape parameter (α) and inverse distance weighting power parameter are dimensionless.

2.6. Air temperatures

As part of the system, maximum, minimum, average and dewpoint temperature observations were detrended prior to interpolation by reducing them to equivalent potential temperature at 1000 millibars (Barry and Chorley, 1998) using surface pressures estimated as a fixed relationship of elevation to surface pressure (Iribane and Godson, 1981). Once predictions were made, potential temperatures were reversed to surface temperatures using estimates of surface pressure at the predicted elevation points.

2.7. Precipitation occurrence and amount

Precipitation is a difficult quantity to interpolate because, due to its discrete nature, it is non-stationary at daily time steps. Therefore, precipitation interpolation is a two-step process: the determination of precipitation occurrence and amount. First, we must define regions where precipitation is likely to occur. Second, we interpolate precipitation amounts contingent on the probability of the occurrence of precipitation at that point. To accomplish this, the OK method uses a combination of indicator kriging (IK) and OK. IK is the categorical equivalent of OK and is achieved by using an indicator variable that represents the occurrence (1) or non-occurrence (0) of precipitation at a given station as an input to OK. The results of IK give predictions that are expressed between 0 and 1 and represent the probability of a precipitation event at a given location. This method has proved useful in improving estimates of non-stationary quantities in other geostatistical analyses (Marinoni, 2003). TGF precipitation predictions were performed by first determining the precipitation occurrence probability (POP) (Thornton et al., 1997) which is comparable to the results obtained from IK. IDW precipitation occurrence predictions were performed using the POP method but replacing the Gaussian weighting function with the IDW function. If the likelihood of precipitation at a given prediction point for a given method exceeds the user-defined probability (0.54 for our application), interpolation of precipitation amount is performed at that point using their respective interpolation method.

2.8. Vapor pressure deficit (VPD) and solar radiation

We estimated actual and saturation vapor pressure (Campbell and Norman, 1998) using the interpolated dewpoint and average daily temperatures and calculated VPD as the difference between saturation and actual vapor pressures. We estimated solar radiation using the method of Thornton et al. (1997) in DAYMET. For

simplicity, we estimated flat-plane radiation, setting slope to zero.

2.9. Cross-validation

To test the system, we performed cross-validation for daily maximum and minimum temperature, vapor pressure deficit, solar radiation and precipitation over the Continental United States for the entire year of 2002, excluding 4 missing days, using OK, the TGF and IDW. For each variable, we estimated the mean absolute error (MAE) and bias to quantify the accuracy and precision of our predictions.

Cross-validation can be computationally demanding for OK if the number of stations used in interpolation is large, as is the case with SOGS. For example, if n is the number of observations, the addition of a single observation used in interpolation represents a 2n+1increase in size of the inter-observation covariance matrix, resulting in an exponential increase in computing time with increasing numbers of observations. OK cross-validation is particularly challenging because each iteration requires the inversion of an n×n matrix of inter-observation covariances. Because the resulting inverted covariance matrix is a square, symmetric matrix, we were able to derive a procedure for calculating the equivalent inverse of the resulting matrix, through row and column removal techniques, which does not require the iterative calculation of the larger matrix inverse. Although many stations in the prediction would have zero weight, this technique is more efficient because it does not require the point-wise filtering of local stations at each prediction point. Depending on the size of the prediction grid, this may be a computationally expensive process. Using this technique, cross-validation time scales linearly with increases in station density rather than exponentially, significantly reducing crossvalidation time.

The matrix inverse routine works as follows. Let M be an $n \times n$, invertible, symmetric matrix (a covariance matrix for our purposes). Once inverted, the M^{-1} matrix is partitioned into submatrices as follows according to the row and column of the inverted matrix that you wish to remove. (For crossvalidation requiring removal of the ith observation, the ith row and column of M^{-1} is removed).

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{A}_{(i-1)\times(i-1)} & \mathbf{f}_{(i-1)\times1} & \mathbf{B}_{(i-1)\times(n-i)} \\ \mathbf{f'}_{1\times(i-1)} & \mathbf{e}_{1\times1} & \mathbf{g'}_{1\times(n-i)} \\ \mathbf{B'}_{(n-i)\times(i-1)} & \mathbf{g}_{(n-i)\times1} & \mathbf{D}_{(n-i)\times(n-i)} \end{bmatrix}$$
(1)

where the *i*th row and column are $[\mathbf{f'} \ \mathbf{e} \ \mathbf{g'}]$ and $[\mathbf{f} \ \mathbf{e} \ \mathbf{g}]'$, respectively. *i* denotes the row and column to remove from the matrix. A new matrix *H* is constructed with the

removal of the *i*th row and column using the submatrices **A**, **B**, **B**' and **D** as follows:

$$H = \begin{bmatrix} A & B \\ B' & D \end{bmatrix}$$
 (2)

and a new vector is formed with the removed column i omitting the intersection value $e_{i,i}$ as follows:

$$\mathbf{k} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix} \tag{3}$$

The inverse of **M** with the *i*th row and column removed, denoted $M_{(-i)}^{-1}$, can then be found as:

$$\mathbf{M}_{(-i)}^{-1} = \mathbf{H} - \mathbf{k}\mathbf{k}'/\mathbf{e} \tag{4}$$

Finding the resulting matrix after removing the *i*th row and column thus reduces to matrix and arithmetic multiplication, division and subtraction operations as opposed to a computationally expensive matrix inversion routine. This routine works for any symmetric, invertible matrix but is used in SOGS on the matrix of inter-station covariances for the OK interpolator.

To quantify the speed increases gained from this matrix inversion shortcut, we performed cross-validation twice, once using this matrix inversion routine and the other iteratively inverting the inter-station covariance matrix with increasing station densities from 100 to 600 stations and measured the time required to complete the calculation for each method. All processing was performed on a Redhat Linux 7.3 workstation with dual 1.6 Ghz AMD Athlon processors and 2 Gb of RAM.

3. Results

3.1. Cross-validation

Results of daily cross-validation for ordinary kriging (OK), the truncated Gaussian filter (TGF) and inverse distance weighting (IDW) for the continental United States for 2002 are presented in Table 2. In general the three test methods performed similarly across all variables. Temperatures predicted with OK had lower

MAE than those predicted with TGF and IDW but no method showed a marked improvement over the other. VPD bias predicted with OK was high relative to the biases in the TGF and IDW. Precipitation occurrence/non-occurrence was predicted with 85% accuracy using Indicator Kriging, 88% using TGF and 87% using IDW. The error matrices for these precipitation occurrence methods are presented in Table 3.

3.2. Resolution change example

The flexibility of the system for use at two widely different spatial scales is demonstrated in Fig. 4. The plates on the left show the results of the one-degree square resolution for the globe for each of the five response variables estimated with SOGS for May 4th, 2003. The plates on the right show the results of a separate run on an 8-km square resolution for the Continental United States for the same variables and day. We see the influence of lack of data on the one-degree resolution product, indicated by a large white stripe through central Africa. This can also be seen in the distribution of observations shown in Fig. 2.

3.3. Cross-validation efficiency test

We found that cross-validation time was significantly reduced using a cross-validation shortcut. If the interobservation covariance matrix was inverted during each iteration of cross-validation, even with only 600 stations, cross-validation would take approximately 1 h. When the matrix inversion shortcut was used, the same cross-validation took approximately 3 min. In general, the process of cross-validation was scaled from an exponential to linear increase in time with the addition of a single station without loss of precision. Fig. 5 shows the comparisons of execution time based on increasing the number of observations.

4. Discussion

Although there are a number of common desktop software applications that can both parse the available

Table 2 SOGS cross-validation results for each of the five key weather variables for the Continental United States for 2002 using ordinary kriging, the truncated Gaussian filter and inverse distance weighting

	Ordinary kriging		Truncated Gaussian filter		Inverse distance weighting	
	MAE	Bias	MAE	Bias	MAE	Bias
Tmax (°C)	1.6	0.03	1.9	-0.01	1.9	0.11
Tmin (°C)	1.9	0.01	2.0	0.01	2.0	0.02
Precipitation (cm)	0.48	0.35	0.49	0.29	0.47	0.27
VPD (Pa)	293.1	-196.6	167.5	7.2	141.6	9.1
Solar radiation (W/m ²)	43.5	-3.4	47.7	-8.7	43.1	-4.2

Table 3
Error matrix for prediction of precipitation occurrence/non-occurrence using indicator kriging (ordinary kriging with indicator variables), the truncated Gaussian filter and inverse distance weighting

	Measured precipitation (%)	No measured precipitation (%)
Indicator kriging		
Predicted precipitation	5	6
No predicted precipitation	9	80
Truncated Gaussian filter		
Predicted precipitation	4	2
No predicted precipitation	10	84
Inverse distance weighting		
Predicted precipitation	4	3
No predicted precipitation	10	83

weather data and interpolate these data to continuous surfaces, these software products lack the ability to perform these processes repetitively or with different mathematical processors without extensive software modifications. Environmental modeling studies often require historical datasets in order to properly account for long-term climatic trends (Cramer et al., 1999). In some cases, these datasets are created daily for over a 100 years, such as those used in the Vegetation/ Ecosystem Modeling and Analysis Project (Schimel et al., 2000). Such datasets would be tedious to create using common desktop software because of the intense amount of user interaction required. Our system can generate such data with minimal initial user interaction over any period of interest or spatial resolution unattended.

Our comparisons between OK, the TGF and IDW interpolation methods show very small differences between the three logics. It is, however, important to note that OK develops interpolation weights not only on the relationship between the prediction point and observation point but rather a combination of those relationships and the relationships between observation points. Clustered stations have their weights reduced because they do not offer independent information to the prediction. This corrects for the uneven or clumped distribution of stations commonly found in spatially explicit point data, eliminating the need to cycle through observation data in an effort to estimate local truncation radii (Thornton et al., 1997). Our implementation is more of an empirical rather than statistical implementation because we used fixed variogram parameters. This ignores one of the strengths of OK: the ability to tailor the interpolator to the spatial correlation of the input observations. For this reason, we would ideally derive our model parameters from a model fit to an empirical variogram calculated from the observed data. In fact, this is part of the program but for our analysis, it was not implemented because we were interested in a more direct comparison of the distance-based interpolators.

Even without this process, we still benefit from ordinary kriging's ability to correct weights under conditions of spatially heterogeneous observations.

Errors for most variables were similar between our three tested interpolators. VPD was the only variable where marked differences in error statistics were apparent. Because the estimation of VPD relies on estimating not one but two temperatures, asymmetries in estimation errors could lead to larger errors in VPD, particularly at higher temperatures. This is possibly why VPD errors were higher even though temperature prediction errors were lower using OK. For example, with similar predictions of dewpoint temperatures between methods, if the error for average temperature were consistently lower with one method, we would underestimate VPD and have a negative bias for that method, as was observed in the error statistics for OK. Equal errors in temperature estimations might represent an equal shift up the SVP curve and thus the estimated VPD might be less biased. As an alternative, we could estimate VPD at each station first and then interpolate the resulting VPD. However, the relationship between elevation and temperature is clearer than the relationship between VPD and elevation. Interpolating temperatures first and using the resulting interpolated temperatures allows us to resolve the topographic influence on VPD. Regardless, all tested methods represent an improvement over previous versions of daily interpolators because they use measured dewpoint temperatures which do not require the estimation of actual vapor pressures based on similarities between dewpoint and minimum temperatures (Kimball et al., 1997).

Errors in daily predictions of precipitation were high for all three methods and little or no differences were ascertainable between the three. Interpolation of daily precipitation values is complicated by many factors. Convective processes in summer create complex patterns of precipitation as compared to broad-scale, frontal winter precipitation patterns resulting in much higher errors in the estimation of precipitation (Comrie and Broyles, 2002). Also, the use of a single truncation radius ignores that there is a different radius of influence for small versus big precipitation events on a daily basis (Skaugen, 1997).

Poor spatial resolution of available meteorological data is a problem for many modeling studies (Cramer et al., 1999; Mummery and Battaglia, 2002) but this constraint is significantly reduced by SOGS. Point data are independent of scale and one can generate surfaces of these variables at any resolution provided that the point data sufficiently resolve the spatial heterogeneity of the process. The data products commonly available to ecological modelers are the actual raster datasets; the initial point data are rarely made available. If the spatial scale of these raster datasets does not match the resolution of other inputs, they are often resampled.

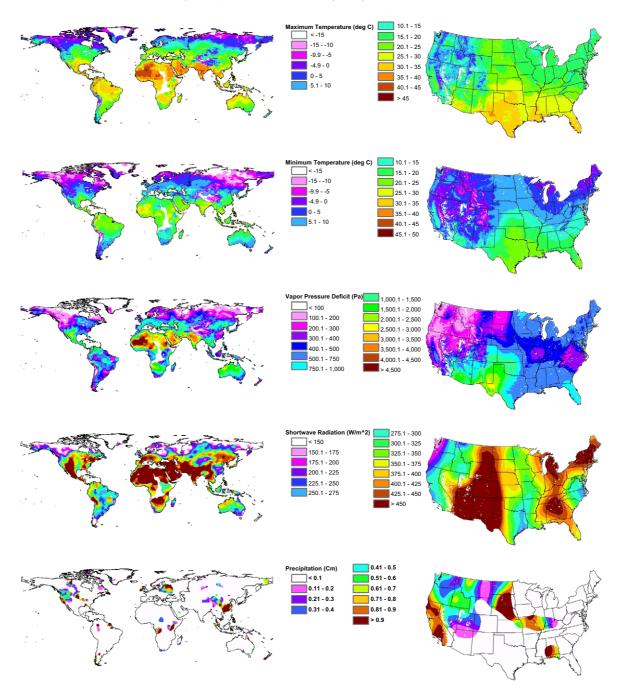


Fig. 4. Example of two different spatial resolution tests for all five variables for May 4th, 2003 using NCDC Global Surface Summary of the Day data. For this test, data were interpolated using the truncated Gaussian filter.

For example, Coops and Waring (2001) were required to resample available raster weather data to match the input of other parameters to their regional ecosystem process model 3PG. Such resampling could significantly bias the results of a model simulation (Pierce and Running, 1995). When point data are stored, one does not need to resample a previously created raster datasets to a new resolution and risk introducing more bias. One can easily switch the spatial resolution of the inputs to

SOGS and generate a new dataset at the appropriate scale based on the original point data, thereby reducing uncertainty in model inputs.

The cross-validation shortcut presented here represented a large increase in efficiency as station counts increased. Without this shortcut, it would have been very difficult to implement cross-validation for OK due to the inordinate amount of time it would have required for cross-validation of 1200 stations. This technique is

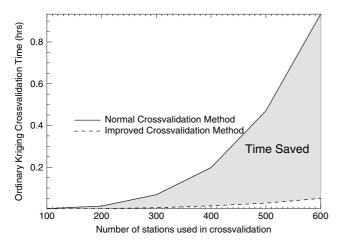


Fig. 5. Efficiency improvements using matrix inversion shortcut relative to the number of stations used in cross-validation of OK showing almost an order of magnitude increase in efficiency between standard OK and our improved cross-validation method. Cross-validation time with the new method scales linearly with increasing station density as opposed to exponentially.

fully generic and can be used anywhere users are required to remove a row and column from an inverted, symmetric matrix.

5. Conclusions

We have detailed a flexible system for the interpolation of spatially explicit point data onto a user specified grid with minimal user intervention. We have presented the implementation of a system that will allow the adaptation to new interpolation methods as they arise as well as a system that is highly plastic in output resolution. We have tested the adaptability of the system to interpolation logic by implementing three separate spatial interpolators and assessed the quality of the data produced by each. We also presented examples of varying the spatial resolution of the output data. This system, we believe, represents an effective way of increasing the application of ecological and hydrological process modeling at a variety of landscape scales.

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